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This is the report of a conference which was initiated by the National Science Foundation's Office of Computing Activities and which explored and summarized current thinking about the role of the computer for undergraduate curricula in the physical and mathematical sciences. The conference focused on deciding which goals of the existing undergraduate curriculum might better be realized using the computer and the extent of revision of present curricula necessary to attain these potential benefits. These were discussed in relation to the subject areas of mathematics, physics, statistics, and chemistry. The discussions emphasized that the computer will alter the curriculum of tomorrow in fundamental ways if educators re-examine the goals of the existing curriculum and begin to actively experiment with this new technology. (GR)

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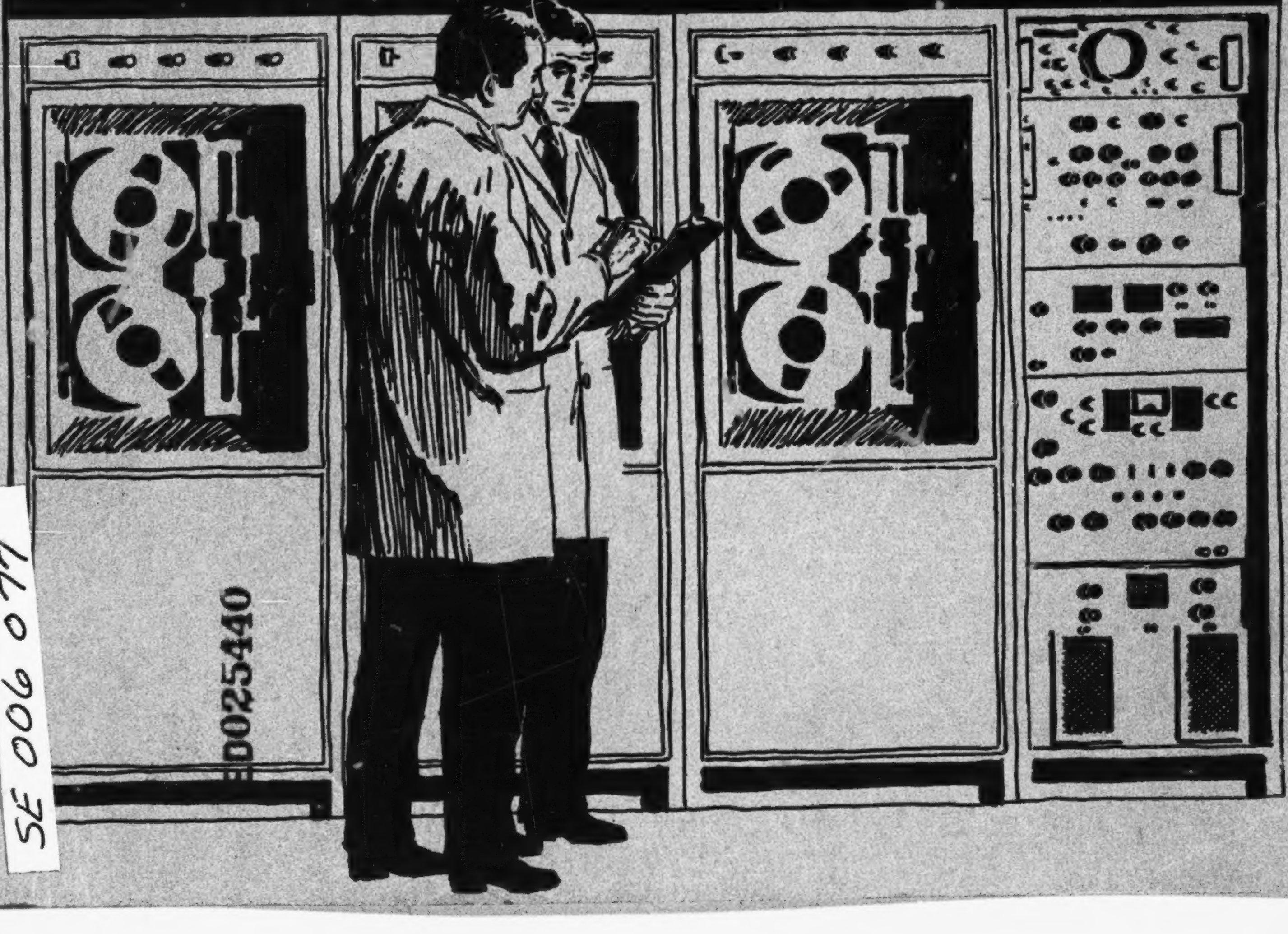
Computers in Undergraduate Education: Mathematics, Physics, Statistics, and Chemistry



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COMPUTERS IN UNDERGRADUATE EDUCATION:
MATHEMATICS, PHYSICS, STATISTICS AND CHEMISTRY

Proceedings of a Conference
sponsored by
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and conducted at
The Science Teaching Center of
The University of Maryland

College Park, December 8-9, 1967

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PREFACE

In 1967, at the direction of the President, the National Science Foundation's newly established Office of Computing Activities undertook an experimental program to develop the potential of the computer in education. This is the report of a short conference, held at the request of the Foundation, on December 8-9, 1967, at the University of Maryland, to explore and summarize current thinking about the role of the computer for the undergraduate curricula in the physical and mathematical sciences. It was intended that this would be the first of several conferences which, taken together, would suggest the extent and directions of change which undergraduate curricula in the sciences, in the arts and humanities, and in professional schools, might experience in the 1970's, were adequate computing services to become more generally available in higher education.

The focal question of the conference was: what goals of the existing undergraduate curriculum might better be realized utilizing the computer, and how extensively would the present curriculum have to be revised to realize these potential benefits? To the extent possible, hardware discussions were to be minimized. Excluded from the conference objectives, also, was an evaluation of the potential impact which the growth of computer science as an emerging academic discipline will have throughout higher education.

To address this focal question twenty-four individuals, representing the four fields of mathematics, physics, statistics and chemistry were asked to meet together (on very short notice) to exchange views on the impact they foresaw computers making in their own undergraduate programs, and to present a summary of their views together with any recommendations they felt were appropriate to NSF in developing its programs. Some of these individuals were active users of computers in their research, while some had little or no contact with computers in any form. Some had already been using the computer in one, or several, undergraduate courses. At the outset some expressed enthusiasm, others skepticism, about possible innovation at the undergraduate level.

The discussants were organized into four panels representing their respective disciplines. Each panel was asked to present a final report of its views and recommendations at the end of the second day of meetings. At a few points a joint meeting of the panels occurred. This proved to be an effective source of stimulation and provided each panel a better opportunity to understand the ideas being developed by other groups. During the second day each panel presented, generally through the voice of its chairman, a summary of its report, following which an open discussion was held which helped clarify and sometimes challenged the views presented. We have tried to convey some of the vitality of this meeting by presenting, with slight editorial changes, both these reports and the discussions which followed.

The meeting was a valuable one for the Foundation's staff. It served to emphasize that the computer will, indeed, alter the curriculum of tomorrow but will do so in very fundamental ways only if educators re-examine the goals of the existing curriculum and begin to more actively experiment with this new technology. We hope the report will stimulate the reader to re-examine his own experiences and evaluate for himself how the computer may enrich the educational experience of tomorrow's student.

We wish to express thanks to the University of Maryland and particularly to Dr. J. David Lockard, Director, Science Teaching Center, for assistance in conducting the conference and in the publication of this report. Thanks are also due to members of the NSF staff, especially to Dr. Thomas M. Gallie, who edited the final report, and to Mrs. R. M. Nieberding who undertook, in addition to many other tasks, the typing and secretarial work involved.

Milton E. Rose
Conference Chairman
September, 1967

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I. MATHEMATICS PANEL REPORT AND DISCUSSION

G. Dantzig
R. P. Dilworth (Chairman)
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REPORT OF MATHEMATICS PANEL

The availability of computers has created new challenges for curriculum development in mathematics. Specifically, the undergraduate mathematics curriculum must be changed to take into account new ways for solving old problems and the host of new problems which have arisen. The Panel feels strongly that students will be enormously stimulated by the introduction of computing into the curriculum; for many it will turn the all-too-often totally passive college experience into one of active participation. It will provide a powerful problem-solving tool, and will enable students to do genuine research at an early period in their training, whereas only the truly exceptional student is now capable of anything worthy of the name research in the classical areas of mathematics. If we can judge from the example of students who have been bitten by the computer bug, their enthusiasm and deeply felt satisfaction comes from their active participation in sophisticated, creative, and truly useful programming projects.

If the basic undergraduate mathematics courses are not appropriately modified to reflect the new points of view which are associated with computer applications in mathematics, these courses will lose much of their relevance for the coming generation of college and university students. This could lead to the unfortunate situation in which instruction in certain basic aspects of mathematics would be incorporated in the programs of other subject areas by default. Thus it is urgent that experimental programs emphasizing this type of curriculum development be initiated and that there be immediate and strong support at the national level.

COMPUTERS AND MATHEMATICS CURRICULUM

It is clear that computers have changed the nature of the solution process in mathematics. In addition to existence proofs, it has now become very important to provide *constructive* methods for obtaining solutions. From a general point of view, many traditional special techniques have been rendered obsolete while the need for an algorithmic approach to mathematical thinking has been strongly reinforced. At the same time, the use of computing methods provides the student with a greater understanding of the concepts involved as well as with greater problem solving ability. Accordingly, it is the opinion of the Mathematics Panel that *computing activities and relevant areas of numerical analysis should be integrated into the first college mathematics course and in subsequent courses when appropriate and natural*.

As a very simple illustration, it is important in the study of calculus that a student understand that a definite integral is a number. The computer can contribute effectively to this understanding. By the use of efficient numerical analysis, he is prepared for the calculation of this number and is not likely to misunderstand the role of the Fundamental Theorem of the Calculus. Moreover, under this approach many of the time-honored techniques of integration which have little pedagogical value can finally be appropriately de-emphasized.

If computing activities are to be integrated in the first college course, the students must be given programming instruction early in their college careers. In the opinion of the Panel, it is not important that this instruction be incorporated in the course. However, programming should be taught in the comprehensive languages of the local computing center and not in a special language constructed for instructional purposes. It is suggested that four to six hours of basic instruction in computer programming should be sufficient to enable a student to make significant use of the computer in his first college course in mathematics.

Applied mathematics courses will be particularly susceptible to improvement through the use of computers and can strengthen and stimulate a student's interest in mathematical problems arising in other disciplines. *Wider experimentation in designing and introducing new courses in applied mathematics, in which computers play a central role, either in classroom instruction, or in individual work on the part of the student, is needed*. In such courses, bold new emphasis should be put on model building and algorithmic solutions of a variety of problems. New areas of applied science can and should be made the kernel of an extensively revised applied mathematics curriculum, augmenting the traditional field of continuum mechanics and its offshoots. Examples of such areas are optimization theory, probability, combinatorial theory, statistical mechanics and applied logic.

The possibilities for significant use of the computer both in the classroom and as a tool for investigations can be illustrated by the following problems in the fields of combinatorial theory and operations research.

Combinatorial theory:

a) Let R_n be the number of non-self intersecting random walks of n steps, starting from zero, on a plane grid. It is known that the limit of $(R_n)^{\frac{1}{n}}$ exists, but the limit has never been computed explicitly. Through the use of high-speed computers, the behavior of this sequence can be studied experimentally. In fact, through such experimentation, a number of guesses about this limit have been made which have had useful applications in physics.

b) Various problems of growth of living systems can be simulated by simple combinatorial structures. Such structures consist, in general, of patterns subjected to random growth, subject only to very simple restrictions. High-speed computers can be used to display the configurations that are obtained by subjecting a system to such a random growth. This type of experimentation can provide the necessary insight for the formulation of reasonable hypotheses concerning the stochastic processes involved.

c) Many of the basic problems are concerned with the enumeration of various types of combinatorial configurations; for example, networks, graphs, etc. In most cases, hand computation is unable to provide suggestive information on the behavior of these numbers. Computers are, if used with sophistication, able to provide the experimental data necessary for the understanding of such enumerations. In some cases, they have already led to precise mathematical results.

Operations research:

a) Many important problems in management science involve the behavior of queues. Through the use of high-speed computers problems concerning queues can be displayed graphically as random events. In this way the observed behavior can be compared with theoretical predictions.

b) The course of computation of the simplex method provides a variety of possibilities for the use of the computer in the classroom or as an investigative tool. For example, it can be used to study the movement of the objective function, the swapping of basic variables, or the effect of changes of parameter.

c) Network flow problems are particularly susceptible to simulation through graphical display using a high-speed computer. As an example of this use, the changes of flow can be studied as one steps through the out-of-kilter algorithm.

In order that student use of computing facilities be effective, it is important that:

1. Subject to very general supervision, the students should have abundant free time to do computer experiments on their own.

2. The facility should provide reasonably fast turnaround time. If possible, consoles should be readily available for student use.

3. A relatively inexpensive display device should be developed which is reasonably flexible and can be used in conjunction with a console without severely restricting the console's operation as a general input-output device.

COMPUTER AIDED INSTRUCTION

In the past, the mathematics instructor has been severely limited with respect to classroom demonstration with student participation. In most cases, the time required for realistic problem solving and graphical representations is simply not available. Potentially the most promising applications of computers to the teaching of mathematics lie in the transformation of mathematics teaching from a completely passive subject to a partially active subject with cooperation on the part of the student.

In the present, relatively undeveloped, state of the art it seems to be clear instruction in the many manipulative drill aspects of calculus could be handled by means of programmed learning techniques in which the computer gives directions to students and monitors their responses. This will require the availability of suitable consoles and appropriate software. It is recommended that a conference of interested persons be arranged to develop a detailed outline for such a programmed learning system for calculus including both curriculum content and *software*. Because the purely manipulative aspects of calculus are frequently neglected in the present calculus courses, a programmed instruction course which would provide these skills without cluttering up the conceptual aspects of calculus could well correct this deficiency.

Computer connected display devices, when used in the classroom, can provide the instructor with a means for illustrating sophisticated mathematical concepts graphically in such a way as to allow for almost instantaneous response to changes in input that might be suggested by the students. Indeed, such a capability in the classroom might elicit more student reaction than is generally possible by standard classroom techniques, even when augmented by canned films. Display devices in the classroom make it possible to integrate the theoretical and computational aspects of mathematics in a way which was not possible before the advent of the computer. That is, examples illustrating theoretical and numerical concepts can be worked out more quickly and modified more rapidly with the aid of the computer than can be done by hand at a blackboard. *It is suggested, therefore, that experimentation with the development of computer connected display devices and appropriate software for classroom instruction in mathematics be undertaken.*

In order to illustrate the uses of such techniques and to give some indication of the kinds of hardware and software required, it may be helpful to examine in some detail the possibilities in an area such as differential equations.

Simple applications in elementary ordinary differential equations could start with display of direction fields for $y' = f(x,y)$ in response to specifying f. Selecting an initial point, with a lightpen, would result in the display (perhaps dynamically) of the appropriate integral curve. Special predetermined f's could illustrate nonuniqueness, i.e., a fan of solutions would emerge. Singular points of $\dot{x} = f(x,y)$, $\dot{y} = g(x,y)$ are ideal display subjects. Stability and its numerical analog which must also be introduced are easily demonstrated by integrating into and out of these singular points. Solution of initial value problems using Picard iteration can be displayed, perhaps using a lightpen to "draw" the initial iterate and thus get some idea of a neighborhood in which a contracting map is defined. The Euler-Cauchy existence theorem can be illustrated by successively refining a mesh using the simple Euler scheme; polygonal approximations could be retained to show convergence if computing equipment were sufficiently powerful. Two point boundary value problems and, as a special case, linear eigenvalue problems can be treated by the shooting technique; contracting maps again enter here but in a simpler way. Behavior of the eigenfunctions and eigenvalues for Sturmian systems are beautifully illustrated by solving appropriate initial value problems with increasing eigenvalue parameter. The oscillations increase as zeros move in from $+\infty$; when a new zero crosses the boundary some special signal is given and the corresponding eigenvalue is shown.

Green's functions can be displayed with the location of the singularity specified by a lightpen; then the response to a force, given analytically or drawn by lightpen, can be superposed. Some playing around like this easily suggests the inverse problem of determining the force so that the solution has desired form - hence Fredholm equations of the first kind. Iterations for Fredholm equations are now naturally suggested and much can be done with integral equations in general.

Partial differential equations are much more difficult to study, not only because the field is so much broader but rather because of the comparably vast amounts of time required for evaluating an approximate solution. Much can be done with the wave equation or even simpler: $u_t = au_x$, to show characteristics, domains of dependence and, for difference schemes, the significance of the Courant-Friedrichs-Lewy stability condition. With $a = a(u)$ and appropriate initial data the formation of discontinuous (weak) solutions can be illustrated. Displays for elliptic problems are more difficult to devise but it would seem that some feeling for the maximum principle, Green's functions and perhaps even the superposition of sources again leading to integral equations could be given by sufficiently clever planning and programming.

DISCUSSION

ROSE:	I'd like to ask whether the other Panels feel that the changes in the mathematics curriculum being recommended here would tend to provide the mathematics training that physics, chemistry and other sciences feel is required.
HULSIZER:	I would respond to that by saying that the physics panel has paid careful attention to earlier remarks made by the mathematics group and we have avoided saying how we thought computing should be introduced to the student for the first time, since they seem to be taking care of that rather well. I think their recommendations would provide physics training the kind of mathematical experience that we would ask. I think on the whole this meshes very, very well with our recommendations.
ROSE:	What is your reaction to the specific recommendation about handling the manipulative drill aspects of the calculus by programmed learning?
MONTROLL:	I think there should be more old-fashioned sitting and doing problems, which tend to be avoided in these new math courses.
DILWORTH:	You understand, of course, we're not eliminating such problem solving. Rather the regular calculus course will be a conceptual

one with the student being on his own to acquire these skills and we only hope to provide the necessary means for doing it without inflicting it on the freshman mathematics instructor.

MONTROLL: I realize that is the easiest way to handle it. On the other hand, I would be happier if you could incorporate this right into the very structure of the course.

DILWORTH: The experiences in math have been that one of the things which makes the freshman calculus course sort of fall apart is that you suddenly have to stop the presentation of the conceptual part and spend some time in practice with integration and differentiation techniques. Many times you lose the student interest at that stage and you never again regain it. It seemed to us that this might provide the way to keep the freshman mathematics course sustained at a high level of interest, particularly if we are able to integrate computing techniques in connection with classroom and problem work.

KREIDER: I guess I don't view this as a very radical change over what we're presently doing -- rather an improvement. We've been accused for some years by our colleagues in other departments of not teaching students an appropriate battery of computational techniques -- [illegible] emphasizing them enough, and they tell us students can't compute. This was at a time when we were not trying very hard to teach these techniques. Subsequently, we tended to eliminate more and more of the special techniques, retaining only the small subset of them required to illustrate the concepts. I would view this now as reintroducing more experience of this kind -- reintroducing it in a way which, in other contexts, has proved very successful. Certainly examples in high schools, and I think also the use in language departments in colleges, suggest that some of the repetitive things you want to teach can be done better by this programmed type of learning. So my view of the entire recommendation is that of adding a further experience with other techniques and, in the course proper, retaining about the same present subset of techniques.

ALEXANDER: I have a little residual skepticism about whether all of these wonderful things can be added and nothing cast out, and I really want to see it proved.

LAX: I would call your attention to the fact that we have mentioned some things that should probably go out -- for example, the special techniques that are frequently included in a course in differential equations. We envision them as going by the board because they just don't need to be used.

MONTROLL: I would really like to see more special techniques. I think there's still a place for doing analysis in various fields.

ALDER: I'm a computer enthusiast -- I use computers, but I think there are many places where mathematical analysis is really very simple, if the student has the right ideas and knows about it. It's too bad that skill is disappearing. You just have to do lots of problems until they're a part of you. You should be able to do analysis just the way you breathe. And the main part of the problem is formulation of the problem, putting in an equation for a computer to solve or simply getting a routine paper-pencil solution.

ROSE: That's still there though, isn't it?

LEES: Yes, we don't propose any place that we're going to replace the thinking and conceptual side.

LAURITSEN: You don't want the math to go into a computer if it can be done analytically.

LEES: That's right and we're very sympathetic -- if it can be done analytically in less than a certain amount of time. It is important to understand the balance -- what you can do easily and what is harder. Many people aren't learning the boundaries.

TUKEY: What thought have you given to the computer's use for algebraic manipulations as opposed to numerical manipulations?

DILWORTH: We didn't give very much thought to that.

TUKEY: I think that's one question that ought to be considered in your report. It might have more impact even than simple numerical manipulations.

DILWORTH: I think that's probably right.

KREIDER: I would like to make one comment with regard to Professor Montroll's remarks. I think the danger in the area of mathematics of rushing in to the computer when analysis is required is much less likely than it is in the area of the sciences. We've had a fair amount of experience in this score and there seems to be very little tendency, even among students where computational facilities are readily available, to make this misuse of the machine.

LAX: I just wanted to add to the discussion of analytic methods that they be applied when they can be applied. I would say one should apply the analytic method if the result of that method is more appropriate to getting results than is a numerical method. This is not always the case.

MONTROLL: One has to have a wide background to know when it is and when it isn't.

LAURITSEN: I think the refreshing thing about this report on the part of the mathematicians is that they are coming spontaneously a long way to doing the kind of mathematics that the other scientists would like to see them do. Let me add that I think it would be arrogant for us to try to tell you how to teach mathematics or even what mathematics to teach. I think you and I, Dilworth, have a long history of discussions in which the physics group has emphasized that what should be taught in mathematics is not physics but mathematics. But it seems to me that the hope is that we have here computational techniques which can bring us much closer together and may very well make mathematics the hand-maiden of physics. I think this remark, however, should not be taken to say that we would like to urge certain kinds of treatments on you or in a certain order. I hope only that this recommendation doesn't get too diluted when it goes out into the world of pure mathematics. I think you're going to have more trouble with your mathematical friends than you have with us.

DILWORTH: I think you're right.

ROSE: One matter that interests me is the following: we didn't invite computer scientists, per se, here, although it is obvious that they would have something of major interest to contribute to these discussions. But I notice that everyone now proposes to treat the computer scientist in much the same way they treated the mathematician in the past. They would just like to use the results of this subject without requiring that the student get any formal training in what the discipline is all about. I wonder whether the computer scientists are going to sit still for this kind of attitude or whether they, themselves, may be pressing for an additional first year course in general, broad areas of computing and computer science.

DILWORTH: In the mathematics panel we discussed this point very carefully. We did not want to intrude on a computer science course in programming in the first year. I don't know if you mentioned it, but I thought we wrote down that we really only wanted something between two and six hours -- not a whole semester's work -- in computer programming. Hopefully, getting the kids onto the computers is probably going to help the computer science program's growth.

II. PHYSICS PANEL REPORT AND DISCUSSION

L. C. Green
R. I. Hulsizer (Chairman)
A. Luehrmann
E. Montroll
M. W. Strandberg

REPORT OF PHYSICS PANEL

A. ELEMENTARY LEVEL

A basic problem for the elementary student concerns the assimilation of basic principles at a time when his command of the mathematical language is still rudimentary. The basic laws of physics are most conveniently expressed as differential equations, but the concepts of differentiation and integration are still mysterious to the student at this level. What he needs in fact is nothing more complicated than the most elementary concepts of a system moving step-by-step from an initial condition to a neighboring one, and this is precisely what a computer does. Given the one attribute of speed, the computer makes it possible for a student to carry out calculations of simple kinematical problems with any desired precision without being confused by the unfamiliar cabalistic symbols of the analytical techniques. The introduction of accelerations and forces becomes equally elementary, and their meanings are presented at the most basic intuitive level.

Following the step-by-step computations of simple systems, it is easy to introduce other force fields - e.g., electric and magnetic interactions - and to extend the discourse to more complex and more real situations. The student can see that the same laws apply and that the difference is only a matter for the computer to worry about. He need no longer regard the three-body problem, for example, as a mystery beyond his ken. The recognition that only arithmetic is needed to extend his command to even the most complicated problems in classical physics should give him an appreciation of the power of the laws he is learning.

With the aid of a computer and the basic principles of force and motion, a student can attack for himself problems of any desired complexity. In the process, he will find that understanding the answers becomes a major challenge. He can now be led to back-track on his over-ambitious approach and to look for means to simplify the conditions to the point where he gets an answer that he can interpret. This process of abstraction, simplification and approximation in a complex situation is just the technique he needs to learn in order to become a physicist. A solution to the most general three-body problem is not likely to provide much insight, but when the student finds that the solution becomes more tractable if one of the bodies is much lighter than the others, or if certain symmetries are invoked, he has learned something about how to reduce a problem to bite-size.

Once a student learns that he can use physics (and computers) to solve real problems, he is in a position to embark upon a form of independent research into fields beyond the immediate demands of a set curriculum. In this sense, the computer serves the purpose of a laboratory, in which he can experiment on problems of his own choosing and with no other constraints than his growing understanding.

In the realms of the very small and the very fast, experimental demonstrations suitable for elementary teaching are difficult to construct. Here the computer offers an attractive possibility as an example of a "perfect" experiment. Visualization of relativistic and quantum effects become possible and suitably constructed displays can be used both for demonstration and for independent examination by the student. The questions he generates through such examination should make valuable starting points for more formal explication in lecture or discussion sessions.

B. INTERMEDIATE LEVEL

When a student confronts theoretical physics at the junior and senior levels, his most important objective must be to develop intuition. At this point he should be in reasonable command of the language and techniques of mathematics and the manipulation of differential equations should no longer frustrate his progress in applying physical principles to real systems. What he needs now is a wide experience with soluble problems and a deep familiarity with the standard solutions. He needs to be able to compare real problems with simple ones and to abstract the essential features intuitively. To move to the new solution, he should command a variety of techniques of perturbation theory, expression in suitable functions and other tools of the trade.

At this stage it is important that the computer not intervene too conspicuously. It can be an aid in computation and visualization, but it must not substitute for thinking or subvert the slow, intensely personal process of wrestling with a problem until one finds a point of attack. Once the problem has been brought to bay, however, it is possible that the computer can be of tremendous aid in displaying the solution, and permitting the student - now the master - to study the effect of such variations as seem interesting to him. Some good examples have been developed in displays of Lorentz transformations and in quantum mechanical scattering problems, where a student can quickly check whether his insight leads him to correct predictions.

C. GRADUATE LEVEL

When a student embarks upon a research program, he quickly finds that the analytic procedures which he has learned do not suffice in the real world. He can apply intuitive understanding and approximation methods to guide his attack on a research problem, but ultimately he has to confront his results with detailed calculations appropriate to the real world. These processes are equally appropriate in his advanced professional courses, and if he can use computer techniques effectively, he can vastly broaden the experience offered in these courses. Just as was the case at the freshman level, he can learn that the power of physical principles is not restricted to idealized systems and, again, that the difference is only arithmetic.

REQUIRED CURRICULAR DEVELOPMENT

A. ALGORITHMETIC APPROACH TO PROBLEM-SOLVING

Students, especially at the elementary level, often leave our courses with the uneasy feeling that physics deals only with problems whose solutions can be expressed as simple, closed-form functions. The search for a solution is, for many, a search among these "acceptable" answers. The computer's skill at performing repetitive operations makes it practical for the first time to solve a vastly larger set of problems at the elementary level. We believe that the student's understanding of physics will be broadened by such an experience and that the development in him of an algorithmic approach to formulating and solving problems is valuable as both a theoretical and a practical alternative to classical methods of analysis. We believe that it will require considerable experience and effort to make this approach a part of our physics courses, and that the introductory courses ought to have priority.

B. THEORY vs. EXPERIMENT

The computer may be a means of bringing the theoretical and the experimental aspects of physics closer together for students at all levels. If the computer or its input/output terminal are in the teaching laboratory it is possible to introduce on a more nearly equal footing, the "real world" of the experiment and the physicists' model of it. A student might change a mass or a spring or a rheostat setting, make the corresponding changes in the programmed version of the theory, and compare his observations at once with the consequences of the theory. Implementation of this use of computers would require a considerable effort to design appropriate experiments, to develop corresponding computer programs and to write new laboratory manuals. It may be best to begin work along these lines in the context of a project laboratory.

C. CERTAIN "PRE-PROFESSIONAL" ASPECTS

Under this heading of career preparation, we list the following problems: a) data handling and b) programs for the more complex problems. In the area of the first of these problems, there is wide recognition of the importance for research of data collection. The importance of data collection is so great that the panel felt that the student should be made aware of the possibilities by the inclusion of some laboratory experience and of some demonstration experiments in the introductory course. In the latter case, direct access to the computer should be available. Equipment for data collection at the level which is likely to be important for the freshman laboratory can be obtained relatively inexpensively, (say $2,000). This could provide a tape punch to record data which could be transmitted to a central computer for the data to be processed. Inclusion in the curriculum will not be a major undertaking. However, the use of such data collection will open up the possibilities for new types of student experiments. In a few cases there are possible effective uses of "data banks" in undergraduate instruction. For example with existence on cards of the NBS tables of the line spectra of the elements, it is possible to reduce substantially the heavy labor of line identification for a stellar spectrum. The possibility opens up an area of student activity which has previously been closed by the amount of semi-repetitive work required before the student had an opportunity to apply judgment or initiative.

A more ambitious undertaking, but also one of potentially great significance, is the on-line tie-in of a computer with apparatus to explore the effects of modifications in the experimental conditions. Some experiments require the reduction of substantial amounts of data to learn how the apparatus is working at a given moment. A case in point is the wire spark chamber. One determines what particles are involved in a given collision by deducing the parameters of the paths from the coordinates of wire pairs in a series of grids. It is instructive for the upperclass or project student to use equipment of this type. It is often not desirable to use a central campus computer for such on-line use both because of the high priority interrupt requirements and the danger of (line) transients. The cost of the necessary auxiliary computer may be of the order of $10,000.

In certain cases, modern knowledge depends in an essential way on the exploration of the possible solutions of the governing equations by the use of computers. Two such fields are stellar structure and evolution and model stellar atmospheres. For a course in such an area, it would be highly desirable to have available a sectionalized program. The student could then be encouraged to study the effects of parameter variations, for example chemical abundance, but more importantly the effects of having the student change certain sections of the program such as those which apply the boundary conditions or a different choice of equations of state or of expressions for the mixing length.

D. A PROPOSED NEW SENIOR COURSE ON MODELING AND MATHEMATICAL METHODS IN PHYSICS

Thought should be given to the development of a senior course on mathematical methods in physics which emphasizes the interplay of analysis and numerical methods in the choice of models used to describe complicated physical situations. Examples should be chosen from a number of different fields, scattering theory, solid state and many body physics, plasma physics, nuclear structure, etc.

Each topic should be developed starting from a single model in which qualitative ideas quickly emerge through simple analytic solutions. Then the models might be made more complicated until a point is reached where the analytical approach becomes difficult if not impossible but by which stage considerable understanding of the physical situation is reached. Finally, computational techniques should be applied to more sophisticated models to obtain quantitative realistic results and to see if surprises developed from the sophistication.

A broad coverage of computing methods should follow from the proper choice of examples. Some should require the numerical solution of differential equations, others non-linear recurrence relations, solution of matrix eigenvalue problems, generation of diagrams and combinatorial analysis, Monte Carlo methods, etc.

Since the easily solvable problems tend to be emphasized in elementary and even graduate courses, students are often shocked when through research they are exposed to real problems. It takes years to develop self-confidence in the definition of models and in decision of how sophisticated a model must be to make it interesting and how simple it must be to make discussible.

If a computer is available for instruction, a course of the type outlined above can give the students some experience in this direction early in their careers and prepare them much better for research work.

In conclusion, the course should not teach a specific branch of physics, but rather should outline the philosophy of the choice of models to describe physical phenomena and the connection of this choice with mathematical methods which are available.

E. LECTURES MODERATED BY USE OF COMPUTERS

Some preliminary exploration with a few problems of interest to physics indicates that the computer can contribute significantly to student understanding and to teaching efficiency. These problems are in topics in which the analytic solutions are cumbersome or intractable and for which a considerable amount of time is required for the student to gain a feeling for what is going on physically in a problem. This is especially true when the problem is obscured with a layer of hard-to-digest functions representing the solution, even though they may have been gained with quite simple analytical procedures. An experienced teacher can illuminate the solution with discussion, but the fact remains that it is difficult to make the student come to the absolute limit of his knowledge without having the student feel some anxiety or lose some confidence in his ability to operate effectively.

The computer can help the teacher at this point if it is used to explore other similar systems much too complicated for analytical solutions or, at least, which have analytical solutions whose written expression gives no simple insight into what is going on. These solutions can be graphed and explored on a computer quite quickly if proper programs and equipment are available and they can constitute an extension of the student's limit of knowledge sufficient to make him feel quite happy with his understanding of the solutions simply available to him.

The problem referred to previously, that of a moving charged particle in complicated electric and magnetic fields, can be used in this way to indicate that the solution the student derives for the case of simple fields in plane or cylindrical geometry connects continuously to a wider field of problems including charge entrapment, and his confidence in his insight or intuition in these problems is correctly enhanced.

Another example would be the investigation of the dispersion surface of the two-dimensional square crystal lattice with nearest neighbor interaction. The solution is simple, and the density of states function may be simply derived in integral form. The properties of the density of states function can be explored by conventional techniques based on a study of the topology of the dispersion surface. This discussion can seem a triumph of virtuosity to the student since it involves piecing together the behavior of the density of states function determined from the critical points of the dispersion surface. However, he can be assisted in his acceptance of these methods by using a computer to generate the whole density of states function for this system and for other similar systems including those with other than nearest-neighbor interactions or with lower symmetry. The basic procedure for studying critical points will then be seen to be generally applicable although with increasing difficulty.

A third example would be an exploration of energy bands in the one-dimensional periodic lattice. The conventional problem explored here is the periodic delta-function potential. The solution for the band edges is simple, although in the form of a transcendental equation. The computer can contribute to the student's experience if it is used to compute the wave functions and band edges for this potential and similar others, such as a truncated coulomb potential, the rectangular well and barrier, and the sine wave. One can display wave functions for electrons within allowed and forbidden bands, the symmetry of the solution at band edges and the continuity of the quantitative properties of the system with changes in shape of the potential. That these latter items are best brought out spontaneously, as the result of discussion in class or of student questions illustrates the power of the computer in extending the lecturer's capability of discussing such topics. Certainly a movie could be made of the properties of a system as explored with a computer, or even single sheets of graphical results could be made. But to afford students a chance to change something and immediately to see the effect is dramatic and would be of great value to students. The sacrifice of this facility will be made with great reluctance once it has been experienced by a lecturer.

The panel recognizes that the generation of these programs and the development of the accompanying dialogue requires massive amounts of faculty time to produce something that has short time use on a one-shot basis. In fact, this technique so reduces the time ordinarily spent by the class on the material thus illuminated, that more material may be covered in the course. To implement this work we recommend that deliberate support by agencies or schools, with some sort of coordination, be given to develop a number of programs, each for a single topic, with an accompanying chapter of text discussing the topic in a manner appropriate to the use of the program. There should also be suggestions of problems for student and classroom notes for the instructor.

F. SPECIFICATION FOR THE COMPUTER FACILITY

We do not wish here to argue the merits of existing or proposed hardware and software configurations. Nevertheless we do feel called upon to point out that all of our discussions have assumed that certain conditions would be met by the facility.

1. Availability. A computer facility must be readily available for use by students. If research is also carried out on the computer, then a set of rules must be established so that student priorities are respected. In view of certain problems in accounting, we believe that the development of computer facilities devoted exclusively to student use should be studied.

2. Turn-around time. Our proposals are not generally practical unless the response-time or turn-around time is of the order of seconds or minutes, not hours.

3. Graphical display. Many of our recommendations, though not all of them, assume a modest graphical output capability. We feel that more experience in using graphical output devices will suggest a far greater reliance upon them in the near future.

4. Languages. We have assumed the existence of user languages which are fairly versatile for performing scientific calculations but which are also easy to learn. Various format-free FORTRAN-like languages seem acceptable.

SOME CONCLUDING RECOMMENDATIONS TO NSF

A. Because of the heavy schedule under which most faculty members operate, we recommend that the National Science Foundation support faculty members in experimenting with and in implementing the above recommendations. Such support would be aimed at releasing faculty members from other duties, hiring supporting staff and paying for computer usage.

B. We urge that the National Science Foundation establish programs specifically inviting production of computer programs and text material introducing such topics as relativity and quantum mechanics at a level suitable for general physics courses. Such material might be in pamphlet form, and should occupy an intermediate position between a simple program outline and a textbook. Possibly the Commission on College Physics could be induced to act as coordinating agency to outline problems and encourage proposals.

DISCUSSION

GWINN: One comment which applies to both the mathematics and physics reports -- there was considerable reference to integration and differentiation and solution of differential equations. This is very important and I realize that you can't put everything in the first two years in the math course. However, they have been giving a fair introduction to linear algebra in the first two years of mathematics at Berkeley and it's very, very valuable from the point of view of chemists and a student seems to pick it up quite readily. Could this be included along with differentiation and integration? We solve many differential equations but rarely do we even write them as differential equations --

usually just as operators with the algebraic solution in terms of matrices. If you go as far as you can in this direction, this would be very desirable.

DILWORTH: I think there is a trend in that direction. For several years now we have included a section we have termed "Sophomore Mathematics - A Course in Linear Algebra Over the Real Field" and it has gone very well and has been quite successful. I think there are many other places getting interested in this too.

RUNNELS: Please say that that course does get to the problem of the diagonalization of the symmetric matrix.

DILWORTH: Yes.

TUKEY: Concerning the period where physicists should study analytical techniques, I believe you mentioned perturbation theory and related topics. One might make good use of symbol manipulation at that point. It can become very awful and there is a practical limitation created by the amount of high school algebra you can do.

ROSE: Are there any further comments about the idea of introducing model-building and related things?

ALDER: I think it's basically the recommendation of the chemistry committee as well. In fact, it seems to be a marvelous way to summarize and bring to a point the training of a chemist or a physicist. Make him work out examples which illustrate the various numerical techniques as well as physical ones in a very concrete way using that tool.

We felt also that this would get him closer to what actually goes on at the forefront in a field in time to decide, perhaps, that he didn't like it. This, usually, he finds out two years into his graduate program. However, he could sample a few of the near forefronts in such a course quite reliably and make a reasonable choice. It's very important that one make this attempt using the computer. Before, one just couldn't have a course like this because it was impossible to spend the time doing it. I view this as an extension of the mathematical-physics course.

HULSIZER: Yes, an experimental laboratory for mathematics.

ROSE: I've heard the suggestion also discussed in the mathematics panel.

KREIDER: I was just going to comment that this almost became one of our explicit recommendations and we discussed somewhat the role of model-building. I think it's intended to be implicit in what we say when we talk about removing some of the time-honored techniques for solving specific problems and replacing them by the direct study of the problem itself. The problem is the model and we would prefer to draw information from the model directly whenever appropriate -- either by theorems and/or by numerical methods. I was rather happy to hear the physicists consider the use of models in two stages -- the first was in their elementary courses where they felt their students did not have the analytic talent to say very much about the models, to draw conclusions, as they put it, to give further insights -- but at least they can use direct numerical predictions there to give the student an appreciation for the comprehension of a particular physical principle. And then later on, they return to models once again and note that sooner or later one has to develop analytic power to deal with models further. I presume your model course would deal with all levels, not just construction of models -- but also appropriate predictions from them.

GWINN: You mentioned a special computing center for students -- I note that Stanford University, for instance, has a special library, in the physics building -- just for its undergraduates. Why not a computing center?

LAURITSEN: At Cal Tech we have a 360/50 system which is almost exclusively for student use. Those of you who have fought the 360 system will realize why it is used only by students. It is in service at the moment -- 25 consoles -- and quite an easy-to-learn language which is used quite intimately in the freshman physics laboratory. It is also used a good deal by the chemists and various other places on the campus. It has been run a good deal, particularly this present year when it's been on-line essentially all the time. And, to date our freshmen have put about five hours apiece in console time on this equipment.

PANELIST: I think it's very important to stop treating students as second-class citizens.

PANELIST: This morning it was suggested that educational uses and research uses of a centralized computer may be incompatible. This might be one way to solve the problem. But, I think rather the problem is not one of incompatibility of these two uses of the computer as much as it is between the incompatibility of the individuals involved. I think one of two things would have to happen -- either you would have to have some agency or institute which sets up proper priorities for student use or else you've got to have two machines -- let the students have one and your researchers the other.

LAURITSEN: Our argument for two computers was partially the fiscal one. How do you account for the time in such a way that the students can afford it? And the other was that the kinds of uses to which the computer is put by students is different from the kinds that a heavy research program puts on it. And you may not just build the two computers the same way.

PANELIST: I'd be interested in the experience of the use of time-sharing with background operations running through it.

PANELIST: Yes, I'm very interested in that, too.

PANELIST: That's a parochial concern of yours.

III. STATISTICS PANEL REPORT AND DISCUSSION

H. W. Alexander	J. Tukey (Chairman)
W. J. Dixon	D. L. Wallace
L. V. Jones	

REPORT OF STATISTICS PANEL

Both in the traditional patterns of statistical education at the collegiate level and in the rapidly burgeoning areas of education that involve data of realistic complexity or data with realistic idiosyncrasies or data with realistic complications, the use of modern computing systems can, and must, transform both the teaching and the effect on the student. Indeed, the computer has already done much to catalyze an increasing flood of change.

The extent of ongoing change is so great, and the depths to which it extends are so fundamental, that we have found it essential to isolate: (1) areas in which immediate action is both feasible and necessary, and (2) planning for a large-scale continuing effort. Accordingly, our recommendations will be similarly divided. It will be essential, in all areas, to involve not only professional statisticians but also those concerned with teaching and research in all of the many using sciences and technologies.

RECOMMENDATIONS FOR IMMEDIATE ACTION

Here we make four recommendations of especial priority:

1. Case studies for exploring data analysis.

2. Sets of data.

3. Exploring feasibility of a current nationally available time-sharing system in undergraduate statistics courses.

4. Support of statistical software packages and systems.

We think it would help with the general picture if we begin with the second major topic, the longer run issue: Establishment of an ongoing program, before dealing with the details of these four recommendations. While there seems to be neither possibility of nor wisdom in the establishment of a single unified curriculum in the area of statistics and data analysis, the gains to be made by broad cooperation and gentle coordination are large and crucially important. Present trends in the redistribution of emphasis and broadening of coverage in undergraduate teaching, already significantly catalyzed by the presence of the computer, make it necessary to move simultaneously in many different ways:

1. Much has to be done, as was noted above, to make available bodies of diverse well-documented and relevant data.

2. The methods and techniques to be applied to these - and other - bodies of data need to be supplemented and re-examined.

3. New textual materials will have to be prepared.

4. Software components making widely different demands upon the computer sophistication of users and upon the character, complexity and power of hardware need to be prepared.

5. All these activities need to be coordinated gently enough to avoid unnecessary road blocks along the way, but firmly enough to avoid unnecessary incompatibilities in the products. (There will be many necessary incompatibilities!)

We have been unable to avoid the conclusion that a substantial organized continuing activity will have to exist to assist on these tasks. It is today too soon to determine either the form or the general terms of reference of such an activity. Two planning steps are needed, and we recommend that the National Science Foundation give very high priority to the support of both:

A. A planning and inquiry activity during the Spring Term 1968, directed toward:

1. Identification of the types of people who should participate in a broader working session.
2. Preparation of background material for such a working session.
3. Inquiry into on-going activities (throughout the country) relevant to the general area.

B. A two-week summer working session, to be attended by 20 to 40 people selected to represent a broad diversity of approaches and fields of interest, whose task would be to recommend the form and sponsorship of a continuing activity, its general terms of reference, and the details of an immediate interim program to be undertaken.

There are many important things which we feel it just isn't feasible to have details on today. And we know, once we plan to have a conference next summer, how long it takes to get things really started. So the four immediate recommendations are thought of as things which deserve immediate attention and for which the general situation, both in our field and on the computing side, is such that they could be proceeded with immediately.

The first one of these is case studies for exploring data analysis. At the same time that we want to use the computer for actually analyzing data, we should not over-look its value as an educational device that can contribute to a student's development without his programming a computer or physically processing the data. In other words, it can help even if he doesn't push a button. One excellent possibility in this direction is the use of the idea of the book for the purpose of a case study. To be specific, a set of data could be taken and analyzed in many ways - some wise, some exploratory, some irrelevant - and then these many analyses reproduced with an accompanying description of the procedures used. Each student would be given a copy of all this material including the original data or, where this is not feasible, at least rather detailed summary statistics. Sets of data of rather different levels of complication will be needed.

What would the student's assignment be? He would study the analyses that have been performed and consider which of them produced more useful analyses, which were wrong or misleading, what adjustments might improve interpretation, and perhaps consider, in the light of their results, which new analyses might be especially instructive. He could, on the basis of several analyses, write up a report on the data and its meaning.

Why would such materials be especially useful and why should the NSF Office of Computing Activities be especially interested?

a) Savings. It can save expense to make one large calculation and reproduce it, instead of requiring each student to program all these calculations himself.

b) Variety and innovation. It gives the student a brisk, well-motivated reason for reviewing and thinking about a large variety of analyses, much broader than he would otherwise ever see in a course in statistics.

c) Profitable complexity. The student begins to see the problem of data analyses in the larger light of something complicated and open-ended rather than tightly knit and closed, a situation where there may not be just one right answer, but many, and where the man with a variety of ideas has more chance to learn.

d) Breadth. It breaks the student and the field of statistics away from the narrowness of small problems with only single statistics applied to one small sample of one-dimensional data.

e) Future development. It may give a common ground for future discussion. Already in statistics there are a few famous sets of data to which we return again and again to show how a particular new method would handle the problems posed. If we had a sequence of good examples like this with the original data available to teachers and students as well as the printout mentioned above, we would begin to find in the literature new and exciting analyses of the same data.

f) Need for many cases. It must be made clear from the above discussion that we do not want to promote just one case study of just one example. We believe that a variety of examples from several fields should be made available. We think that support should be made available for developing these case studies along with reports of their use in courses. No doubt teacher's manuals will be useful.

The second one of the four recommendations is labeled "sets of data." A set of 20-30 well-documented examples of data problems which can form the basis for illustrating statistical methods. (We're now moving on to material to which methods can be applied and applied live as opposed to material on which methods have been applied in wide variety.) In selecting these problems it would be well to provide diversity at least in the following dimensions for these problems as examples:

1. Number of observations or cases
   Small, medium, large
   Should the range be 3 to 20,000?

2. Number of variables
   Is the feasible range 1 to 1,000?
   We've not had time to set and make recommendations on this but think these questions help to indicate what we're thinking of.

3. Types of variables
   Categorical, scores, measurements, etc.
   Do we need a finer breakdown?

4. Completeness of the data set
   Should this range from 20% to 100% with a few at about 98% complete?
   Should the completeness be known or unknown?

   (This is just a little "jargon" and it implies that, of the cases that you might expect to have or the variables that you might expect to have on a case, all are rarely there. Partial absence produces a variety of stressful questions as to what you should do.)

5. Stratification
   Single, multiple ordered or categorical, etc.
   Is this a separate classification or an alternate under types of variables?

6. Data sources
   Real world, generated data of various forms.

7. Areas of application
   Physics, chemistry, biology, social sciences, etc. Quite a lot in the etc., we think.

8. Suitability for a variety of statistical techniques
   The data description should be sufficiently detailed that the suitability of some alternate techniques can be judged.

We recommend that the National Science Foundation support the gathering and documentation of a diversity of examples. We believe this will support activity needed in this area. It is not a trivial task to get this sort of thing together and get it done.

The third recommendation calls for exploring the feasibility of a current nationally available time-sharing system in undergraduate statistics courses. It is intended or proposed to select as participants some 40-50 teachers of undergraduate facilities at 40-50 colleges and universities. At the time of application, each would become committed (a) to utilize the computer in an undergraduate statistics course during the 1968-69 academic year; (b) to participate in a summer workshop preparatory to such use. In return, all accepted candidates would be assured the full financial support of costs associated with this exploratory program, including rental costs of consoles or a console at his college or university, travel and per diem costs (as well as a stipend) for the summer workshop, costs of duplicating special course materials, and costs of preparing reports.

Summer workshops would be organized profitably at at least three colleges or universities regionally spread out, each planned and designed by faculty at that institution. Workshop duration might be three weeks. The teacher-participants would become familiar with the console and an associated language, particularly for analyzing data and performing statistical computation. They also would be trained in the use of statistical packages that are available on the system for standard statistical analysis.

They would learn to use random samples from a given distribution, generated by the machine, in order to study sampling distributions empirically. In addition, they would become acquainted with a wide variety of case-study examples, for each of which a repertoire of statistical analyses had already been produced.

A central coordinating function of the workshop would be the dissemination of written materials serving to describe possible units of course study, documenting ways for using the computer console in connection with each unit, either in the classroom or as out-of-class student exercises. In particular, sample sets of data would be made available in connection with each possible course unit - sample, not simple. New units might be devised by subgroups of participant teachers, and some allied programs would be developed by the subgroup, documented and made available to all participants.

All participants would be expected either to use in their courses a subset of these course units, or to develop and make use of some they might construct on their own.

The sponsoring agency might agree to assume all costs of the summer workshops. Progress reports would be sent by all participants to the sponsoring agency and made available for study to all participants.

The essential point here is that, in many institutions and in present circumstances, the only way we can accelerate computer involvement is to make available a console. There are enough alternate nationally available console systems to keep this from being a one-system proposal. It would be a sensible opportunity to be of assistance to various campuses, and it seems to us that, if something is going to get started with the smaller institutions -- those that do not have computers -- this is the only way to do it.

The fourth recommendation deals with the support of statistical software development and implementation. Two areas deserve special mention here:

1. The development of statistical software packages designed for educational use in early courses in methods

and theory is an urgent need.

2. Immediate support should be provided for the development of innovative uses of the computer in statistical analysis including interactive and graphical consoles, file handling capabilities, shared data and program libraries, etc., so that more powerful computer support can be provided in the near future.

The need for specific discussion is greatest in connection with the first of these.

Most currently available statistical software packages are directed toward large-scale data analyses and research and are not conducive to effective use on a broad scale in undergraduate courses in statistics. No single package will ever suffice and an immediate program for the support of diverse individual and group efforts to develop packages is essential. Among important dimensions for varied approaches are the access methods and the type of course uses. Interactive and batch systems, with input/output via teletypes, high-speed printers and display consoles will all remain important in the foreseeable future.

Theory courses will have needs distinctly different from methods courses and great differences within choice of methods will require different approaches. Difficulties in making software available at installations other than the home installation are huge and will remain so. These difficulties can be reduced by care in the design and implementation of a system, and supported developments should make great efforts here. Immediate support should be provided to institutions to implement appropriate systems developed elsewhere, as they become available. In the future, workshops on these software developments may be desirable. The immediate need is for financial support of individual efforts to develop systems.

DISCUSSION

DILWORTH: Gentlemen, I have the impression that you are proposing an attack on a very broad area. Now, statistics in universities is tremendously widely scattered -- departments and everything else. I gather that you are proposing sort of a broad-sided attack on this. What is the argument for this rather than a pilot attack on a portion of the area to see how it goes?

TUKEY: Well, I don't think the area has portions. In an era with the computer coming in, you are going to find, insofar as you're talking about analyzing data, that the more things you try to bring together, the more sense things make. The various elementary courses that will come from a process of evolution aren't going to differ widely in techniques. They may differ in applications. There is difference of opinion in the panel as to whether all of the elementary courses in statistics are going to come together or whether they will all break apart and get taught in the individual departments. But this is a secondary matter.

DILWORTH: But, don't you have a specific recommendation -- for example, I forget the figure -- but something like twenty realistic examples from different fields?

TUKEY: I think that number's going to go up as you start working on it. The first step is twenty realistic large examples where we don't have any now. Two hundred would be a nice figure, but let's get twenty first.

DILWORTH: The twenty is a pilot study?

TUKEY: Yes.

MONTROLL: Yes. What's starting to show up very clearly in my mind and, I suspect many of you have already realized this, is that whereas the use of the computer for elementary instruction is a sort of nice thing -- maybe it's better, maybe it's worse than programmed instruction books or lectures -- at the more sophisticated level, the upper-class or the purely graduate student level, one would be able to do very realistic problems as instruction examples. Now one tends to give very simple things as compared to what is being done in the forefront. However, instead of the student through his thesis activity getting on the forefront of one little bit of a science, he would now be able to get to the forefront of the whole field and do very realistic things with his courses. Perhaps that should be a keynote.

PANELIST: Is it in order for me to make a motion that this be adopted as a keynote for the report?

ROSE: It's on record.

Now, there's one thing I don't understand completely. It's the recommendation about an available time-sharing system being adopted throughout the country. Could you amplify on that?

TUKEY: If you're going to do something which involves some serious retreading -- and this does -- in a number of institutions -- retreading one man per institution, it just isn't feasible to retread one man one way, another man another way, and so on -- until you have fifty different men all trained fifty different ways. I think it might be perfectly possible, if you followed this recommendation and set up two or three summer workshops, to try two or three different nationally available computer utility systems, if there were two or three which proved out when you looked at them. But a workshop has got to be big enough to be viable and the people in it have got to use the same system. Otherwise, you don't have an effective workshop.

ROSE: I'm trying to understand this -- these statistical packages -- somehow you have in mind making them available through the computing centers at the individual campuses.

TUKEY: Let's mention names and take one example. BASIC is available as part of a computer utility through General Electric Centers generally around the country. It's a fairly easy system to learn -- you can do quite a lot with it. Supplementing the statistical side of this a little would not be too hard.

ROSE: Here you're talking about the summer workshop?

TUKEY: I'm talking about what the teachers are going to learn to use. And that has to be a language, a system and a set of statistical subjects. The present state of the computer utilities appears to be that they will accept supplements to their systems to be accessible on request. So, it doesn't matter if you're in South Carolina or Nebraska. You wouldn't be using the same computer; you would be making telephone calls to different central locations.

PANELIST: Do you have in mind something like a man producing a large program and coming into a workshop and telling teachers, "This is all my program can do"?

TUKEY: No, no, no. We aren't going to do anything of that sort. We're talking about the kind of teachers here who teach statistics at smaller institutions, typically less than a couple of thousand, who have probably never used a computer themselves, who have a real barrier to get over in learning to use the computer and coming to feel they can do things well enough to stay somewhere ahead of their students. It's the more elementary things they need to use.

PANELIST: Such as BMD, the set of programs developed at UCLA?

TUKEY: BMD is specific. Any BMD programs I've seen are oriented to the research angle. We're talking about things which are oriented to the first course in statistics.

PANELIST: Are you going to produce it in BASIC then?

TUKEY: Lyle has had more specific experience with what is presently available on BASIC, I think. Do you want to try to answer this question, Lyle?

JONES: The presently available system features teletype consoles, and sub-routines may be prepared using either a version of FORTRAN or the BASIC programming language. A package of statistical routines may be prepared in FORTRAN and called by the user for analyzing data input at his teletype console. Or, the user may write his own special-purpose routines in the simpler BASIC language. We envision teachers coming to the summer workshop to learn how to use this system. Programs -- statistical routines developed at the workshop -- could be distributed to all participants for use in their college classes. Upon return to their colleges, participants would continue working at the teletype consoles there, before courses begin. They utilize this console in their classrooms with their students using some of the materials which were generated at the workshop's setting. As they gain more confidence they may develop other materials using BASIC. Also, their students may generate routines for analysis of data. The concept is one that is primarily oriented toward colleges which do not enjoy at the present time local computer facilities at all comparable to those available to many of us in our universities.

ROSE: Well, I guess the most common kind of thing we'll need is for a person to go back to this institution and get on the small computer which his institution has.

TUKEY: You're talking about an upper-class person compared with our proposal. We're talking about the people who, for some reason or other, don't have a computer or don't have access to one at their institutions. We're really trying to say that here's something you can do at the grass roots. And, let's go do something there as well as provide things coming down the line.

ALEXANDER: Are we going to be able to arrange the conference this summer and the course in September or October? I don't know how these things move, but consoles are growing awfully scarce at the moment.

ROSE: I should mention in connection with what you're saying that we are planning this year to start a number of pilot regional computing activities. The idea here was to take various colleges which either don't have computing or need a variety of new dimensions in computing and to enable them to get computing service remotely from an institution which has more computing capacity available and more experience. The kind of thing that we see developing is that there will be a variety of different kinds of computing capability on different campuses. I think now I understand better what you said. I had thought that you were proposing that one system should be developed which contained all of the packages that everybody wants.

TUKEY: We have strong feelings against this; we would favor two or three diverse systems. We were talking about the elements of the situation, with no implication that you can do all of the things you want. We have one other thing -- I don't know about time, but Dr. Alexander had a recommendation -- one with which we generally concurred, but one so broad that we thought it ought to be brought up out of context of the panel. So, if you could recognize him --

ROSE: Certainly.

ALEXANDER: This is a proposal for regional, multidisciplinary conferences on the educational implications of the computer. Such a conference is envisioned as appropriate for the institution involving, let us say, fewer than 2,000 students. Some of these schools would have a computer on campus; others would have one or more consoles; still others would not yet have any such hardware on hand. All, however, would be actively interested in exploring the ways in which education (both in-class and out-of-class) can be enriched and facilitated by computer usage.

The disciplines invited would cover the whole range of the sciences, including physical, biological and social sciences as well as statistics and mathematics.

(1) Such a conference would hope to accomplish the following: Present specific examples in

which the computer is used to accomplish something that could not readily be achieved without it; for example, an interactive learning process taking place at the console.

(2) Discover what computer facilities are presently available at the institutions represented, and what program packages are needed and/or available to accomplish certain educational objectives.

(3) Specify certain of the problems that urgently need to be solved, in terms of equipment, programs, training, textbooks, manuals and the like.

Now, this is envisioned as involving, let us say, several states and an invitation would go out to colleges within a certain range to attend a two-day conference. I would think of it as being parallel to what has occurred here in some respects except that it would not be making broad proposals or be necessarily innovative itself, but would consider the immediate feasibility of the kinds of things we have talked about here for the institutions that those people represent.

ROSE: One of the ideas here would be to cover many fields.

PANELIST: Do you see this conference as having a consultant come in and tell them what kinds of things could be available -- in case they have no idea of how to use this? Or would you expect them to apply their own initiative?

ALEXANDER: Yes, I would imagine the speakers, the leadership of the conference, would be people of the kind you are suggesting.

IV. CHEMISTRY PANEL REPORT AND DISCUSSION

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REPORT OF CHEMISTRY PANEL

The Chemistry Panel was unanimous and enthusiastic in endorsing the use of computers in undergraduate education. We can easily think of many areas in which the computer can now be used very effectively to enhance greatly the student's understanding of chemical systems. A limited number of such examples are listed in Appendix I. Chemistry is a field ideally suited for the use of large digital computers. We have sophisticated theories and complicated mathematical developments which are applicable to our real systems. Very often both the mathematics and the chemical systems are so complex that to obtain any theoretical predictions or any comparisons between theory and experiment, it has been necessary to make many approximations in order to get any results. The power and usefulness of the theory is very often negated. Large digital computers are rapidly changing this situation by making possible valid calculations on real and complex systems. Our chemistry students need to learn these methods.

Many of us have been very concerned by the small number of our chemistry students who are well trained in mathematical and physical methods. One of our problems is that beginning students see very little of the mathematical or physical aspects of chemistry. Too often theoretical chemistry means to them empirical correlations. Consequently by the senior and graduate level, many of our students who have special mathematical talents are drawn into some other field. We believe that the introduction of computers for the solution of chemical problems at the freshman and sophomore level will have a tremendous impact on mathematical chemistry by letting the students at an early level see what more advanced chemistry holds for them.

Computers already make important contributions to graduate education in chemistry at the research level, but there has not yet been widespread use of the computer in undergraduate chemistry education. It is an exciting possibility to be able to introduce computers at the lower level. Computer solutions often facilitate a completely different approach to a problem, and it is essential to introduce these methods at the earliest possible time.

Before it is possible to make very effective use of computers for undergraduates, there are several important and formidable problems which must be solved. These problems may be broadly classified as those involved in: (a) introducing the computer to the student and teaching him to write programs, (b) introducing the computer and programming to those on the faculty who have not already had experience with the technique, (c) obtaining a set of suitable computer-oriented problems, a set of laboratory experiments in computer-instrument interaction, and a set of programs which are ready to run and can be used to study chemistry with little or no programming, and (d) obtaining the necessary hardware.

COLLECTION OF COMPUTER-ORIENTED PROBLEMS IN CHEMISTRY

An important step in the solution to these problems would be the preparation of a set of suitable computer-oriented problems to be used in various classes in chemistry. Such a compilation would be an extremely important catalyst to initiate a wide-scale introduction of the computer to the chemistry undergraduate curriculum. This collection should include problems for which the student will do all of his numerical analysis, write his own programs and study the results. At the other extreme, it should include completely prepared programs for which the student inserts various input parameters and observes the calculated chemical consequence. It should also include all gradations between these two extremes. It should include some laboratory experiments in which a small computer or fast interactive terminal with analog-to-digital (voltage) and digital-to-analog converters are connected directly to chemical experiments.

Some of the specific advantages of such a collection would be: In many chemistry departments only a small fraction of the faculty is actively involved in computing. This presents a problem in that, while a computer may be used to handle the routine tedious part of a problem, regardless of what type of solution or numerical methods are used, far more effective and complete solutions may be found by using a type of numerical analysis which is best suited for computer solution. It is a valid analogy to relate an optimum computer solution to a successful and somewhat tricky forward pass or end run in football, which is in contrast to a routine adaptation of existing solutions, or in the analogy to football, to a routine rush through center. In most of our courses, much time is spent on developing closed form solutions which are amenable to hand calculations. Some of these are very important to develop concepts and "intuition", but most become obsolete when a computer is available. It would be unreasonable to expect the non-computer-oriented instructor spontaneously to develop computer solutions for his course, but a good compilation of problems, examples, and thoroughly tested programs would give the instructor the opportunity to study the material beforehand, test it, and then use it in his class. We believe this compilation of exercises is almost of parallel importance to the availability of computer equipment.

Such a book of exercises would also greatly assist the computer-oriented instructor. It takes a tremendous amount of time to work out suitable exercises and to develop a set of thoroughly tested programs. Even problems, in which the student is going to supply all of the mathematical analysis, are very time-consuming because prior to class assignment the instructor himself must completely work out and program the problem to be sure it will be suitable for the class. Usually many more problems are tested than are eventually used. This is in contrast to the situation found in giving an existing course. New problems are constantly being introduced, but there is always a large backlog of standard, pre-tested problems and a few innovative problems each year represent only a nominal load. The second type of problem, in which the student uses prewritten programs, requires even more time. It is essential that these routines be written with extreme care and that they be as nearly fool-proof as is ever possible.

This endeavor requires a tremendous amount of time, and it is important to pool our efforts so as to maximize our results. In order to pool our efforts effectively in the development of such a set of exercises, it would be well to designate an editor and a group of interested people and to give financial aid for collecting and developing a set of computer-oriented problems. To initiate computer usage it is very important to have an instructive set of problems which have been completely tested and are at the same time exciting and realistic illustrations. This set of problems should include examples from all branches of chemistry and should include as wide a variety of numerical methods as possible. Some possible examples are included in Appendix I.

It would be well to hold one or two short meetings during the summer for participants who are contributing to this problem book. Meetings should be held at an institution which has good computer facilities with remote terminals where programs can be tested, modified, and further developed. The resulting book should be paper bound to emphasize its temporal nature. Although we consider the book to be our most important recommendation, it is intended only as a catalyst to initiate the program. It should be superseded by the problem set of each individual instructor after he becomes sufficiently familiar with the use of the computer in undergraduate instruction.

The National Science Foundation can assist in the implementation of this computer-oriented curriculum by making available to the faculty who are writing and initiating this program, high-level programming assistants and other personnel required to develop and initiate and test the necessary basic programs and descriptions. In most institutions this will be a continuously developing curriculum and the continued programming assistance will be of tremendous value.

It will also be essential that universities and their faculties cooperate in developing the modifications to the curriculum. It is important for universities and colleges to recognize and make available the time required by the faculty members to create, design, develop and evaluate such a program. In chemistry the use of the computer will very likely be distributed throughout all courses, rather than in a single course. A large degree of cooperation will be needed between the faculty setting up the computer usage program. Universities should not put the entire burden of financing upon the Federal Government, or as a corollary, the faculty should not have the sole responsibility to finance everything through grants from the Federal Government. It is important that faculty members are not overloaded with other teaching and committee responsibilities during the development period.

EDUCATION IN COMPUTER USAGE

Another problem of concern is how to make the introduction of the computer to students and faculty who are not already familiar with its usage. With chemistry students this problem can best be solved by the execution of one of the recommendations of the Mathematics Panel. Our work in chemistry would be greatly facilitated if their recommendation, that courses in elementary mathematics make use of the computer and numerical methods in teaching elementary mathematics, were put into practice. Not only would mathematics become more meaningful to these students, but they would be better prepared to study chemistry and other physical sciences. In most universities at the present time, computers are introduced in several courses. It seems that regardless of whether it is a junior, senior or graduate course, there are so few students who have had prior contact with computers that it is necessary to introduce computers and programming from the beginning. As a result, the limited amount of class time is gone before any effective use is made of the computers.

It is essential that students learn programming at the earliest possible time. Chemistry courses should concentrate not on programming but on the application to setting up, solving of chemical problems and to the later interpretation of the results. But, if necessary, a very short (one unit) course may be needed to insure that all freshman chemistry and chemical engineering majors become familiar with programming.

It has been the experience of most of us that students require very little formal instruction in the details of computer programming. There is a high barrier to getting them to write their first very simple program, but from there on, they very rapidly expand their programming capabilities and fluency if a computer is readily available to them. Remote terminals, to which the students have ready access, can be of tremendous value in developing their curiosity and in expanding the student's programming knowledge.

Where they have been available, remote terminals have also been found to be of great value in introducing the computer to the faculty members who are unfamiliar with computers. This has been found particularly true where portable units are available to be plugged into jacks in faculty offices.

TYPES OF COMPUTER USAGE; HARDWARE SYSTEMS

The availability of the proper hardware systems will do much to enhance the instructional use of computers in chemistry. In chemistry there is a wide variety of tasks which a computer will be required to perform. The optimal hardware for each of these will appear quite different to the user. These various functions may or may not be handled effectively by any one of the different types of computing systems available.

The most common use of the computer by undergraduates will be for writing short programs, or for inserting parameters into library programs to investigate the chemical consequences of certain models. Rapid response is essential so that the student can interact and supply new and altered chemical situations (new input parameters). By this method the student is able to use the computer somewhat as an experimental tool with which to study various chemical models under dynamic conditions. If the student is forced to wait a day or so between entering a set of parameters and getting the results, the continuity of the experiment is lost. The excitement of the rapid computer interaction is replaced by frustrations. We, therefore, believe that remote terminals are highly desirable for student use. This particular value of the remote terminal is in addition to that previously discussed in relation to the students and faculty learning about computers.

Our panel spent considerable time discussing various types of remote terminals, including teletype systems with fast turn-around (1 to 5 minutes in the worst case), interactive teletype systems, and display systems. All of us felt that display systems had many instructional advantages. Graphical methods have been widely used in chemistry. The presentation of ideas, whether it be to students in a classroom or to fellow scientists at a meeting, is greatly facilitated by graphical methods. A simple set of curves has a far greater impact on audiences than do long lists of numbers. There is no reason to believe that the graphical display of computer output will not also speed comprehension of output results.

Remote terminals utilizing graphical displays do present certain difficulties. They are expensive, both for terminal hardware and for computation time. The display system must be interactive. In most cases the operating program for each console must be either resident in core, or swapped between the working core and either a fast drum or an extended core memory. In either event, a large amount of computing power is tied up with each remote console with a display system.

However, several systems have been recently developed which are considerably less expensive. They are built around an ordinary storage oscilloscope and digital-to-analog converters. One of these, the Culler-Fried system, uses a particularly small amount of resident program and core swapping. It uses its own programming language which is very close to ordinary mathematics (much more so than FORTRAN). This makes it especially attractive for the beginning students. The question remains as to how gracefully the students will make the transition to more complete and complex programming systems. It is very important to obtain this answer as soon as possible. At the same time it is important to test fully the educational value of display systems and to determine what price in computing facilities display systems are worth.

A second type of remote terminal is the teletype interactive terminal. Here each character from the teletype is tested and used by the program as it is typed from the teletype. This system has all the disadvantages of the display systems in that the entire program must be resident in the core or, alternatively, a large amount of computing power is tied up in core swapping. Our panel was quite dubious of the advantage of a single character interactive system.

One problem with both display systems and interactive teletype systems is that they conflict with another very important use of computers. In advanced courses, such as quantum mechanics, students should work with fairly large and long-running programs. Also, a large fraction of the education of a graduate student is in research. In graduate research, the full computing power of our largest machines is needed. If these machines are used in interactive systems, they must always be ready to interact. They must have programs in core or going in and out of core on a millisecond time scale. As such, they are not available for large calculations. Our panel felt that this was too high a price to pay for an interactive teletype system.

Another type of teletype system can be made very compatible with running large programs. In this system, programs are written and stored on disk files (preferably with fixed heads, i.e., one head per track). When the programmer wishes, he may call for compilation or execution. He then waits until the current job is finished (or after 30 sec. or so, the current job is put off on disk to be restarted after completion of the waiting programs); then his program is run. The output is placed on disk to be slowly put out at teletype speed. This system using only one-line core buffers for teletype input ties up very little core storage, and does not involve the large overhead found in fast core-swapping systems as needed by the interactive computing systems. It is applicable both to small and to large computing systems. A more detailed description of the operation of such a system is given in Appendix II.

ON-LINE DATA COLLECTION AND INTERACTIVE CONTROL OF CHEMICAL EXPERIMENTS

In addition to the use of the computer for chemical numerical analysis, there is a very important use in chemistry for on-line data collection and interactive control of chemical experiments. These experiments make possible the execution of experiments which were completely impossible a few years ago. Data can be extracted from signals which were previously completely buried in noise. Control can be made more exact, faster and more reliable using a computer. It is important for our students to see and learn these techniques. The most likely way this will be done is to use a small digital computer ($20,000 ± $12,000 at present) in the physical chemistry laboratory, with facilities for students connecting it to various experiments.

Depending upon local conditions, the small computer may be replaced by an interactive remote terminal with digital-to-analog and analog-to-digital facilities. In making this substitution, caution should be exercised to be sure that the remote terminal will be available at all times and that it can handle fast data rates. Often interactive systems have response times of 10 to 100 milliseconds. This is satisfactory for teletypes but not for on-line data collection where good but small systems can collect over

10,000 voltages per second. Another alternative is the use of a somewhat larger computer. On-line data collection from experiments is combined with on-line program collection from teletypes. Again caution should be exercised if it is planned to have the local computer transmit programs to a central large computer. Local conditions should be thoroughly studied first. How fast can programs be accepted? How will the data be transmitted? How will the computers be coupled? Who will write the system program in the large system to accept the foreign computer?

COMPUTER ASSISTED LEARNING

There are several other possible uses of computers in chemical education. A large category is contained in what is known as "Computer Assisted Learning" (CAL) or "Computer Aided Instruction" (CAI) or "Computer Based Education" (CBE). These terms are not well defined, and any use of the computer in the chemistry undergraduate program may quite properly be called CAL.

Sometimes these terms have been used to refer to the interaction of a student with a computer which is used primarily for information retrieval and information transfer processes. In these uses the responses of the student are often compared with the prerecorded responses which are to be expected, or the student is given bits of information which he requests from the files which have been previously stored in the computer. The panel was unimpressed with what has already been done in this form of CAL in which the computer is little more than a "page-turner" for the student.

On the other hand, CAL offers unexplored opportunities. The real problem is the generation of appropriate learning situations coupled to a computer with well-defined educational objectives in view. There is no reason why a computer must stand alone (as a page-turner), isolated from texts, laboratories, specially prepared manuals, audio-visual materials, or indeed from the instructor himself. Rather the effective use of the computer must integrate many of these learning resources.

Since there is so little available experience in CAL in chemistry, we have found differences of opinion as to the probable success of CAL techniques in specific applications. For example, it is clearly possible to devise programs to assist students in learning to balance chemical equations. The situation is ideal in the sense that many instructors now must spend enormous amounts of time and energy on drilling students who desperately need the self-confidence in mastering these simple problems. The computer can be a much more patient drill-master. On the other hand, it is not clear that it isn't faster for the student to count atoms, and it isn't clear that there wouldn't be more mistakes in typing than mistakes in balancing equations. Such possible applications, however, can and should be tested by experiment in small groups of students before we would be in a position to recommend heavy developmental expenditures.

More sophisticated examples are not hard to imagine which might be more challenging. An example involving the thermodynamic properties of a diatomic molecular system is included in Appendix I although some members of the panel define CAL too narrowly to include this conveniently within its purview. One could even go to a further extreme to suggest that some of the most effective CAL situations may be found when the student is interacting directly with a computer-controlled experiment.

It is likely that CAL offers real opportunities in presenting chemically interesting situations matched to a student's state of achievement. The panel's limited experience suggests that CAL programs now in existence are totally inadequate. It would thus seem that exploratory research, especially involving creative new approaches, is justified. If individuals with interest, imagination, and demonstrated scientific ability can be persuaded to work in this area, their research deserves support. Thus, while a majority of the panel was opposed to wide-scale implementation of CAL in the present state of the art, it did recognize that there are unrealized possibilities in this area, and that research should be carried out and supported and encouraged, especially if carried along with a strong arithmetic program.

OTHER USES

The introduction of computers for undergraduate use would carry some additional benefits. The instructor should use the equipment and programming assistance to aid in compiling and making out grades, to study and analyze the results of quizzes, etc. Again, this should be not to automate grading, but to permit the instructor to better analyze, relative to a student's background, why the student missed certain questions. There are many imaginative uses to which the computer could be put in addition to relieving some of the drudgery of the instructor's paper work.

We have restricted this report to undergraduate students, but our recommendations would greatly aid the graduate students also. By the time the student reaches graduate courses he has an excellent background in mathematics and numerical analysis and he has learned enough chemistry to use these methods to great advantage. The undergraduate use would be during scheduled hours during the day. The graduate students could use the equipment at night (and possibly during parts of the day) at very little extra cost. Large computers almost always run 24 hours a day. For small computers the only cost of 24-hour use is power and maintenance on peripheral equipment. The central processor maintenance is almost independent of whether or not it is used.

Any system set up specifically for undergraduate education would also be expected to be used by graduate students for research purposes, when the system is not being used for course work.

RECOMMENDATIONS

There seem to be three general types of situations to which computers can make a valuable contribution. They are very different in philosophy. These types of problems and philosophies may be contrasted by classifying them as: (a) Problems in which arithmetic presents a formidable barrier between setting up a physical model and seeing the end conclusions, (b) Problems in which the students learn about the methods and use of on-line interactions between a small computer and chemical instruments, (c) Problems involving the use of a computer to store large files of information to be compared with student responses. Our panel was unanimous in placing its main emphasis both upon on-line instrumentation, and upon the use of arithmetic problems for teaching chemistry to college and university students.

There are many possibilities of numerically oriented problems (also logic problems) for chemistry. A few specific examples will be given in Appendix I.

Our general hope was that students learn enough programming in the elementary mathematics courses to get them started. They would also learn enough numerical analysis to make a good start, and that our efforts should be primarily concentrated on the interface between chemistry and numerical analysis and on the interface between the results of the calculations and chemistry.

In summary, our panel recommends:

1. That an editor be appointed to collect and to develop a set of problems which would be available for each level in the education of the chemistry student. This editor would contact a group of experienced (in both computers and education) people from all branches of chemistry. With National Science Foundation support they would each develop a computer program illustrating chemical principles and numerical methods, drawing from their own fields, to be included in a book as a chapter with a

pedagogically suitable write-up.

2. That projects be supported in which a small computer would be purchased for use in on-line chemical experiments. This is an implementation of the above recommendations where problems involving connecting computers to experiments, data handling, and data analysis are covered in the book to be used in a junior physical chemistry laboratory.

3. That National Science Foundation funds be supplied for high-level programming and/or engineering assistance and partial faculty salary support in order to initiate the use of the problem book. The programmer and/or engineer is needed to develop additional numerical problems, to connect remote hardware for student use, including graphical displays, and to aid on-line experiments. The faculty support is needed because of the large amount of time involved in creating, designing, developing and evaluating such a program, so that he should be released from all duties during the initial phase of this effort except the continuation of his graduate research. Of course, the necessary hardware to implement these systems should be supported as well.

4. That computer aided instruction not be widely implemented at present because the state of the art is not sufficiently well developed. We do recommend, however, that support be made available in this area for both hardware and software to those individuals who have the interest and abilities to make imaginative and fruitful progress in research and development in computer assisted learning.

APPENDIX I

This appendix contains several examples of problems of the type which might be introduced at various levels of chemistry.

Example 1. On-line data collection from a calorimeter experiment in a junior-senior course in physical chemistry laboratory. This is intended as an introductory experience in on-line experiments.

An experiment often done in physical chemistry is to measure a heat of solution in a calorimeter. Small heats are involved and small temperature changes are measured. There is a steady heat leak to or from the calorimeter which must be considered in the calculations. The temperature change is measured using a thermister in a Wheatstone bridge (or a resistance thermometer in a Mueller bridge), and the calorimeter is calibrated by adding a measured amount of electrical heat. Student equipment is usually a bit more primitive than research equipment. Batteries drift and fluctuate in voltage and, for example, during the calibration period, the student must work hard to get three temperature measurements and two current and voltage measurements. In practice, the two power measurements usually show a considerable discrepancy. Repeated calibrations give larger disagreements than would be desired.

The proposed experiment would be to have the student do the measurements with conventional technique. Afterward he would repeat the experiment using a small computer equipped with a digital-to-analog (voltage) and an analog-to-digital converter, and a multiplexor so as to connect the A/D converter to several voltage sources. He would use three of these inputs: one for the output of the temperature bridge, one for the voltage drop across a standard resistor so as to measure the current in the calibration heater, and the third for the voltage across the calibration heater. Using the real time clock interrupt for timing, he would measure up to 100 temperatures and electrical powers per second, continuing on for several minutes. (Data would be worked up during the progress of the experiment so as not to exceed the core capacity of the small computer.) Signals from the computer would start and stop the heating cycle at the end of the experiment. During the experiment, up to 60,000 measurements would have been taken. As the experiment progressed, the power measurements would be worked up into a numerical integral and by digital filtering, the large number of temperature points would be collapsed to a smaller number which could be stored. This more tractable set of data would be printed by a teletype in the laboratory (if the computer were remote) and the temperature vs. time would also be plotted on an ordinary strip chart recorder using the D/A channel of the computer. The computer would then be used in a more standard manner to determine the steady heat leak and in general work up the data.

In the first few years of this experiment, we would probably furnish the data collection program. Later, when students were more familiar with computers, the students would write their own programs.

Example 2. In studying complex chemical bonding, a very useful method is the one electron, linear combination of atomic orbitals, molecular orbital method. This method contains many approximations, many of which are balanced against and nearly cancel other approximations. Although absolute quantitative significance should not be attached to the method, it does present a very good picture of what is going on when chemical bonds are formed. It gives quite realistic relative effects when bonding situations are altered. The one electron functions or orbitals produced by this method form a very useful basis for understanding and setting up more complete electronic calculations. The computations are extremely fast and simple even on a small computer.

Using the example of a set of electrons in a molecule, such as styrene, the problem would be set up using as basis functions one P_z orbital on each atom.

Using the approximations of this method, we would write the Hamiltonian operating on this basis set as,

$$H \varphi_i = \alpha_i \varphi_i + \sum_j{}' \beta_{ji} \varphi_j$$

where φ_i is the i^{th} basis function centered on atom i, α_i is an empirical constant which represents the ionization energy of an electron on atom i, and β_{ji} is another empirical constant which is linearly related to the strength of an isolated bond between atoms i and j. In this representation the student can easily write the Hamiltonian matrix. The diagonal elements would be the ionization energies of each atom and would reflect the electronegativity of that atom. The off-diagonal elements would represent any bond or partial bond, depending upon the model the student is setting up. Thus, the student could set up the Hamiltonian for any arbitrary geometry and any type of atoms, with partial bonds connecting any pair of atoms.

The Hamiltonian would then be diagonalized to give the solutions of the Schrodinger equation. The diagonalizing transformation T, in $T'HT = E_{diagonal}$, could then be used to find the density of electrons at each atom i; for each orbital k (density = T_{ki}^2) and the contribution to the bonding of each pair of atoms, i and j, $(T_{ki} T_{kj} \beta_{ij})$. These would be returned separately for each orbital, k, and then summed over all occupied orbitals and the results printed. The student could repetitively enter different α's and β's and so dynamically study the effect on the model of varying various parameters (atoms or geometry).

This exercise would be useful at several levels. The sophomores could use it as a prewritten program, in which they experimented with input parameters. The program should type out a warning that quantitative nature of the answers should not be taken too seriously. In the junior, senior and graduate years the students could write their own programs. Graduate students could then add transformations such as rotations by an arbitrary angle, reflections, inversions, etc., and investigate the symmetry properties of the resulting orbitals and compare them with those expected from group theory. They could also construct group theoretical character tables from a sufficient number of sets of orbitals of different types. They could see dramatically the results of using incomplete basis sets. There are many other variations of this exercise possible.

Example 3. The student is given a black box program in which the dynamic motion of about 100 disks can be followed. He can change the initial positions of the particles, the velocity of the particles, and the size (density) of the particles. Possible experiments are:

1. State of Matter (Freshman)
   - (a) solid at high density - investigate how far a given particle leaves its location by observing its position
   - (b) liquid at lower density - repeat and show that a particle reaches all parts of the container - measure the diffusion coefficient by how fast it does
   - (c) gas at still lower density - repeat and contrast with a liquid by observing how long the particle is confined to the same set of neighbors

2. Approach to Equilibrium (Senior)
   Start all particles with the same velocity but in random directions. Plot the velocity distribution after some time, calculate the Boltzman H function, and see how it behaves as a function of time, show that the final distribution is Maxwellian.

3. Fluctuations (Junior)
   Put all particles in the left half of the box initially - measure the number in the left half as a function of time. Why does the initial part of this curve illustrate irreversibility? What are the fluctuations? Calculate the probabilities of their magnitude. Do your fluctuations conform to these?

Example 4. This exercise is to find all possible products of a reaction in organic synthesis. It is patterned after an actual program used in research by Professor W. G. Dauben and Edward Debus of the University of California.

In their work a product was isolated after a certain reaction. By a molecular weight determination and a C, H, and N analysis it was found to have a certain number of each type of atom. Knowing the empirical formula, they thought of about four possible compounds for the identity of the product. In order to avoid overlooking any possibility, they wrote a computer program to find all possible compounds with this empirical formula. They put in a few constraints as to structure but they were taken by surprise when the computer program returned over 700 possible compounds. The 700 compounds were all real compounds but most could be eliminated as products of the reaction under study. Various constraints based on the actual chemical reaction under study, such as ring size and interconnection of rings, were added, one at a time, until the computer program also gave only four possibilities. Thus, they did not find any overlooked species, but they did learn much about how their "chemical intuition" worked. They found they were putting many actual constraints in their thinking. They learned that they actually had used these ideas of logic in a much more formal manner than they had realized when they made their initial "intuitive" search for possible reaction products.

This exercise may be adapted in many possible ways for freshman through graduate levels.

Example 5. A program might be devised leading the student through the computation of the enthalpy and entropy of a gaseous diatomic molecule and its atomic components, e.g., Cl_2 and Cl atoms. The statistical problem is relatively easy to state; the molecular model of a rigid-rotor, harmonic oscillator, contradictory though it may appear, is good enough for calculations of adequate accuracy; a minimum of molecular data is needed and can be built into the program for a variety of molecules and atoms. As an extension, thermodynamic data can be included: heat capacity as a function of temperature, latent heats for phase transitions, and the same quantities, i.e., the enthalpy and entropy of the gas, can be calculated from these data. The program could be written pursuing the same logical sequence the instructor might follow in guiding the student to a solution of the problem. It should be keyed to the student's text for basic concepts, derivations and formulas; checks and tests should be built into it as appropriate with recommendations for action in case the tests or checks show the student has missed the path. Again, there is no reason why the recommendation could not be given the student that he consult either other books or an instructor if he fails at any point; there is no reason for the computer to stand alone any more than there is for a student to work totally alone in a laboratory with no instructor present to advise and assist him as needed. The scientific objective of this program would be a computation of enthalpy and entropy as a function of temperature and pressure, a graphical display of these results, and a comparison with real data; the pedagogical objective would be not only the demonstration to the student of the application of these techniques to a chemical problem, but also the addition to his self-confidence in the application of these rather complex ideas. Once the computations are available, chemically more interesting questions may be posed, e.g., the equilibrium between the diatomic molecules and atoms, the influence of temperature and pressure on the state of this equilibrium, the significance of enthalpy and entropy changes in determining the equilibrium situations, etc.

An objection may be raised that this problem is trivial; it is little more than using the correct formula, plugging in the correct data. This objection is the traditional one raised by many non-chemical chemists who feel that only derivations of formulas lead to real "understanding", and the objection has been countered often by those who feel that no problem is worth studying unless it leads to comparison of derived results with genuine experimental data. It is not our purpose to argue this point, but rather to indicate extensions of the above problem which might prove valuable. The fact is that such problems have real pedagogical value.

Although there is no reason why the derivation of formulas required could not be programmed directly, there seems little more reason for repetition through such a program than for repetition through a lecture since the derivation is likely contained in the text, or could be written in a hand-out, anyway. But if the derivation is deemed important, it might be carried through with a parallel example, e.g., the distribution over energy levels of the harmonic oscillator, the selection of the "most-probable distribution" (if that is the argument followed), the probability of this distribution, and the significance or limitations of the whole argument. Actually, as is well known, this exercise leads to a far-from-trivial problem which might cause the student to worry over the entire formulation of the statistical arguments.

Alternately, if the existence of the formulas is accepted, the student could be led to consider the numerous factors involved in them and the sensitivity of the results to molecular parameters, and thereby develop some intuition in their application. For example, the relative contributions to the energy and entropy from translation, rotation, vibration, and electronic excitation could be displayed for a host of different molecules and atoms relying on the existence of data available in the computer memory or, if desirable, in tables provided to the student with the program.

Example 6. Prewritten Programs for Use in the Chemistry Curriculum. The following examples are arranged in approximate order of appearance in the curriculum. Notice that most could be used both for teaching purposes and as a tool in the laboratory. Also notice the rather heavy dependence on display equipment.

a. Fluid behavior. Using simple empirical equations of state with variable parameters, the student learns about properties of real and ideal gases, condensation, critical phenomena.

b. Rate equations. For simultaneous first order rate equations, the time dependence of the various concentrations are presented, showing the effect of different starting conditions and rate constants.

c. Curve fitting. A program to determine a least-square straight line through data points would illustrate data analysis as well as the determination of activation energies, dipole moments, intrinsic viscosities, etc.

d. Third Law entropy. The principle of numerical integration would be illustrated with examples drawn from thermodynamics, including third law entropies, activity coefficients, etc.

e. N.M.R. From coupling constants and chemical shifts supplied by the student, the N.M.R. spectrum would be displayed. For comparison, the spectrum could be given to various orders of perturbation.

f. Quantum mechanics. The ground state wave function would be displayed for a one-particle, one-dimensional problem, with the potential (of reasonable form) supplied by the student.

g. Variational principle. The student would experiment with different trial vectors (functions) to gain a feeling for the important characteristics of an eigenvector (eigenfunction) of a symmetric matrix (kernel).

h. Statistical mechanics. The student would supply a spherically symmetric intermolecular potential and receive as output the temperature dependence of the second virial coefficient and the low-density radial distribution function.

Example 7. Classical Scattering from a Central Force. Except for some relatively simple examples it is fairly difficult to describe the nature of the trajectories which result when particles are scattered by a central force. The parameters which describe the problem are, in addition to the potential which may be rather complicated, the initial velocity of the particle and the angular momentum. The numerical solution of the differential equations in r and θ as a function of these parameters is rather straightforward and would provide, when displayed graphically, a way for a student to investigate the nature of the scattering problem for a variety of cases. This kind of computer program used in conjunction with some of the more usual mathematical discussions of scattering would give the student a better physical feeling for the behavior of these systems.

Example 8. Orthogonal Functions. The theory of orthogonal functions plays an important role in many areas of chemistry, particularly in quantum mechanics; however, because of the numerical difficulties involved, few students have had the opportunity to actually carry out some of the calculations which are possible. For example, most every student learns how to do a Fourier analysis except he never in practice actually does it; the closest he comes is the determination of a few of the coefficients but seldom does he ever, for example, reconstruct the original function. This is obviously a simple case suitable for fairly inexperienced students but there are others, for example, transformation theory in quantum mechanics, for which actual examples could be worked out. We look at this kind of use of the computer as a mathematical laboratory where a student can explore the mathematics of a chemical system much in the same way he might explore the chemistry of a chemical system in a conventional laboratory.

APPENDIX II

A possible useful teletype system using FORTRAN will be described in this appendix. There would be two distinct areas on the disk reserved for each teletype. As data is received from the teletype, it is stored in a one-line buffer in core (one line for each teletype). When a carriage return is detected, the line goes into part of a FORTRAN compiler to check syntax. If an error is not detected, it is placed on disk. If an error is detected, a line editor is called and the error flagged on the user's teletype. The user corrects the error by insertion, deletion, or replacement of characters in the line, or by shifting part of the line to insert a space, or by complete replacement of the line. These edit features are also available before the user types a carriage return. After checking syntax the line, if good, is placed on disk. After completion of the program, compilation would be called for (EOR key) and usually higher order errors would be detected (transfers, etc.). These errors would be corrected by intermixing, deleting and adding statements from the disk and teletype under control of the user. New statements would be checked for syntax and edited. The revised program would be written on the second area of the disk. The program would be edited repetitively, going from one area of the disk to the other, until there were no errors. The binary program would be placed on the unused area of the disk and the user would assert any number of three options: (a) return the source program, (b) return the object program to the paper tape punch of the teletype, or (c) execution of the program after entering the data. (This description is very similar to an editor now implemented on the College of Chemistry S.D.S. 910 computer at the University of California, Berkeley. The differences are that control and input come from only one console typewriter. The entire FORTRAN compiler is used, giving syntax and all other errors. There is no disk or drum. Instead two tapes are now used for storage. The line editor is not called for errors but is used in the second stage where statements are edited and intermixed from magnetic tape, paper tape, and typewriter. The system runs time-shared with data collection and on-line control of several laboratory experiments. The FORTRAN execution phase is not yet implemented.) Similar systems exist commercially.

Such a system ties up very little core for the teletype system, and carries no large overhead found in fast core swapping systems as needed by the interactive computing systems. It is applicable both to small systems and to large systems. In large systems, a small external computer would very likely collect data (programs) from many teletypes, contain the editor, and syntax checker, and handle the disk storage. When a program was ready for compilation or execution, it would be transmitted to a large computer for running. The output would be sent to the small computer for return to the particular teletype as soon as it is produced in the large computer. The user should have the option of taking some output, examining it and making a decision as to whether the program should continue with or without new input data. The user would insert these control points in his program in the usual way, by printing as output a request for input. The system would automatically transfer the program to disk and run the next program in the job stack. When the input data is received by the small computer in the proper format, the job would be put back in the input queue and in turn restored to operation.

The user should be able to program for a moderately large amount of output. After it is on disk file in the small computer, the user should then have the option of deleting n lines of printing at any time. This should be done without destroying the file. This would give the user the option of spot-checking data, examining it to see if it would be necessary to print the entire file. (This is in recognition of the fact that most printing is used only for spot-checking results, and that printing is an expensive part of present-day computation or, alternately, that a large amount of printing on a teletype is very time-consuming.)

DISCUSSION

LAURITSEN: I have a comment which was induced by the remarks about laboratory computing equipment. There have been a number of admonitions about what we should be doing. One of these has to do with separate classification of computing equipment. This has caused a good deal of agony both in research laboratories and in educational institutions. You can spend $10,000 on a piece of apparatus as long as it doesn't have a memory on it. If it has a memory, then you can whistle for it. I think you know the problem. The other is a similar fiscal problem which has to do with the cost of computing time. This is, in fact, one of the arguments for having two computers on a campus -- because under present regulations it is necessary that all users pay the same rate for the use of the computer. This has a tendency, I think, to inhibit the use of computers by students. When we can get around this fiscal problem, we might be able to attack more basic problems.

(The discussion at this point elaborated upon relationships between certain recommendations of the Chemistry and Physics Panels. Because many of the comments, particularly those by Professor Strandberg, were later incorporated in the final version of the Report by the Physics Panel, the discussion is omitted here for the sake of brevity.)

ROSE: Well, I certainly won't attempt here to summarize this afternoon's discussion. It has been wide-ranging and will prove to be very useful for all of us at NSF. I'd like to conclude the formal meeting but encourage further conversation and discussion.

I would like to express our appreciation to the University of Maryland for hosting this conference and for making such charming and effective members of its staff available to us. And, thank you all very, very much for having come to help us so willingly.